Reliability Science, Entropy and Applications to Corrosion-Fatigue

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Our Overall Research Objectives

- Describe materials damage resulting from failure mechanisms within the irreversible nonequilibrium thermodynamics and information theory frameworks
- Improve understanding of the coupled failure mechanisms such as corrosion-fatigue including confirmatory tests
- Further strengthen the foundation of reliability sciences in the context of the classical thermodynamics, statistical mechanics and information theory
- Explore applications to Prognosis and Health Management (PHM) of structures



Motivation

- Markers of damage: changes in crack length, elastic modulus, micro-hardness, ultrasonic wave, and electric resistance, weight loss,....
- Macroscopic fatigue markers are detectable mostly after expending 80 ~ 90 % of life



 Basaran et al., and Bryant et al. have pioneered thermodynamic concepts to assess damage.

Motivation (Cont.)



[1] Anahita Imanian and Mohammad Modarres, A Thermodynamic Entropy Approach to Reliability Assessment with Application to Corrosion Fatigue, Entropy 17.10 (2015): 6995-7020
[2] M. Naderi et al., On the Thermodynamic Entropy of Fatigue Fracture, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 466.2114 (2009): 1-16



A Thermodynamic Interpretation of Materials Damage



Second Law of Thermodynamics: In an isolated system, entropy will always increase until it reaches a maximum value.



Second Law of Thermodynamics (Statistical Mechanics Version): In an isolated system, the system will always progress to a macrostate that corresponds to the maximum number of microstates.

Interpretation of Mechanistic Damages in terms of the 2nd Law

All damages resulting from failure mechanisms share a common feature: Dissipation of Energy.

Dissipation: a fundamental determinant of irreversibility can be described well within the context of the nonequilibrium thermodynamics.



Thermodynamics as the Science of Reliability



Why Entropy? Entropy is independent of the path to failure ending at similar total entropy at failure Entropy accounts for complex synergistic effects of interacting failure mechanisms Entropy is scale independent



An Entropic Theory of Damage



An entropic theory follows^[1]:

Failure occurs when the accumulated total entropy generated exceeds the entropic-endurance of the unit

- Entropic-endurance describes the capacity of the unit to withstand entropy
- Entropic-endurance of identical units is equal
- Entropic-endurance of different units is different
- Entropic-endurance to failure can be measured (experimentally) and involves stochastic variability
- In this context we define Damage as: $D = \frac{s_d s_{d_0}}{s_{d_E} s_{d_0}}$

Total entropy generation, s_d , monotonically increases starting at time zero from a theoretical value of zero or practically some initial entropy, s_{d0} , to an entropic-endurance value, s_d



^{8 [1]} Anahita Imanian and Mohammad Modarres, A Thermodynamic Entropy Approach to Reliability Assessment with Application to Corrosion Fatigue, Entropy 17.10 (2015): 6995-7020

Total Entropy

• The variation of *total entropy*, dS, is in the form of: $dS = d^r S + d^d S$.

 $d^r S$ = exchange part of the entropy supplied to the system by its surroundings through transfer of matters and heat: $\frac{d^r S}{dt} = -\int^{\Omega} J_s \cdot n_s dA$

$$d^{d}S$$
 = irreversible part of the entropy produced inside of
the system: $\frac{d^{d}S}{dt} = \int^{V} \sigma dV$.

- Divergence theorem leads to: $\frac{ds}{dt} + \nabla . J_s = \sigma$, where, *s* is the specific entropy per unit mass.
- An Expression of Damage, *D*, according to this theory $D|t \sim \int_0^t [\sigma|X_i(u), J_i(u)] du$

J=entropy flux; X = entropy force, σ =entropy generation/unit volume/unit time

Surroundings $d^r S$ System $d^d S > 0$ $dS = d^r S + d^d S$





Total Entropy Generated

• Entropy generation σ involves a thermodynamic force, X_i , and an entropy flux, J_i as:

 $\sigma = \Sigma_{i,j} X_i J_i(X_j) ; \quad (i, j=1, \dots, n)$

For near equilibrium condition interactions between $mu^{l+inl_0} \stackrel{discinction}{=} \sum_{j} L_{ij}X_j$ processes is captured by the Onsagar reciprocal relations define forces and fluxes. $J_i = \sum_{j} L_{ij}X_j$ For example for Fatigue (f) and Corrosion (c)

 $J_c = L_{cc}X_c + L_{fc}X_f$ and $J_f = L_{cf}X_c + L_{ff}X_f$

 $[L_{ij}]$ = Onsager matrix of phenomenological coefficients

• Entropy generation of important dissipation phenomena leading to damage:

Thermal energyDiffusion energyPlastic deformation energy $\sigma = \frac{1}{T^2} J_q. \nabla T + \Sigma_{k=1}^n J_k \left(\nabla \frac{\mu_k}{T} \right) + \frac{1}{T} \tau: \dot{\epsilon_p} + \frac{1}{T} \Sigma_{j=1}^r v_j A_j + \frac{1}{T} \Sigma_{m=1}^h c_m J_m (-\nabla \psi)$ Chemical reaction energyExternal fields energy

 J_n (n = q, k, and m) = thermodynamic fluxes due to heat conduction, diffusion and external fields, *T*=temperature, μ_k = chemical potential, v_i =chemical reaction rate, τ =stress tensor, $\dot{\epsilon_p}$ =the plastic strain rate, A_j =the chemical affinity or chemical reaction potential difference, ψ =potential of the external field, and c_m =coupling constant *, **

*D. Kondepudi and I. Prigogine, "*Modern Thermodynamics: From Heat Engines to Dissipative Structures*," Wiley, England, 1998. ** J. Lemaitre and J. L. Chaboche, "*Mechanics of Solid Materials*," 3rd edition; Cambridge University Press: Cambridge, UK, 2000.

Examples of Force and Flux of Dissipative Processes

 $\sigma = \Sigma \quad V I (V) \cdot (i = 1)$

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$0 - \mathcal{L}_{i,j} \mathcal{L}_{i,j} \mathcal{L}_{i,j} (\mathcal{L}_{j}), (i, j-1, \dots, n)$			
Primary mechanism	Thermodynamic force, X	Thermodynamic flow, J	Examples of materials damage process
Heat conduction	Temperature gradient, $\nabla(l/T)$	Heat flux, q	Fatigue, creep, wear
Plastic deformation of solids	Stress, σ/T	Plastic strain, $\dot{\boldsymbol{\varepsilon}}_p$	Fatigue, creep, wear
Chemical reaction	Reaction affinity, A_k/T	Reaction rate, v_k	Corrosion, wear
Mass diffusion	Chemical potential, $-\nabla(\mu_k/T)$	Diffusion flux, J_k	Wear, creep
Electrochemical reaction	Electrochemical potential, \tilde{A}/T	Current density, i_{corr}/z	Corrosion
Irradiation	Particle flux density, A_r/T	Velocity of target atoms after collision, \dot{v}_r	Irradiation damage
Annihilation of lattice sites	Creep driving force $(\tilde{\boldsymbol{\sigma}} - \omega \boldsymbol{I})/T$	Creep deformation rate, R	Creep

Table From: Amiri, M. and Modarres, M., An Entropy-Based Damage Characterization, Entropy, 16, 2014.

Entropic Approaches: Fatigue Mechanism



Information Theory Based Entropy







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Information Entropy



AE information entropy



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Experimental Setup and Measurements

- Stress and strain: load cell and extensometer
- Crack length: Optical microscope

- ✤ AE: two AE sensors
- Temperature: thermocouple





Entropic-Based Damage from Corrosion-Fatigue (CF)

• Oxidation and reduction reactions of metallic electrode, M, under CF: $M \leftrightarrow M^{z_M^+} + z_M e^ 0 + z_0 e^- \leftrightarrow R$

O = Certain oxidant in solution resulting in formation of the reduction product R.

- The entropy generation results from:
 - Entropy flow to the surrounding
 - Entropy generation from:
 - Corrosion reaction processes
 - Electrochemical processes
 - Mechanical losses
 - Diffusion losses
 - Hydrogen embrittlement losses







Entropy Generation in CF

• Contribution from corrosion activation over-potential, diffusion over-potential, corrosion reaction chemical potential, plastic and elastic deformation and hydrogen embrittlement to the rate of entropy generation:



T = temperature, z_M =number of moles of electrons exchanged in the oxidation process, F =Farady number, $J_{M,a}$ and $J_{M,c}$ = irreversible anodic and cathodic activation currents for oxidation reaction, $J_{0,a}$ and $J_{0,c}$ =anodic and cathodic activation currents for reduction reaction, $E_{M_{act,a}}$ and $E_{M_{act,c}}$ =anodic and cathodic over-potentials for oxidation reaction, $E_{O_{act,a}}$ and $E_{O_{act,c}}$ =anodic and cathodic over-potentials for oxidation reaction, $E_{O_{act,c}}$ =anodic and cathodic oxidation and cathodic over-potentials for the cathodic oxidation and cathodic reduction reactions, α_M and α_O =charge transport coefficient for the oxidation and reduction reactions, A_M and A_O = chemical affinity for the oxidation and reductions, $\dot{\epsilon}_p$ =plastic deformation rate, τ =plastic stress, \dot{D} =dimensionless damage function A_M the elastic energy, and σ_H =entropy generation due to hydrogen embrittlement.

Imanian, A. and Modarres. M, "A Thermodynamic Entropy Based Approach for Prognosis and Health Management with Application to Corrosion-Fatigue," 2015 IEEE International Conference on Prognostics and Health Management, 22-25 June, 2015, Austin, USA

Corrosion Fatigue (CF) Experimental Set up

- Fatigue tests of Al 7075-T651 in 3.5% wt. NaCl aqueous solution acidified with a 1 molar solution of HCl, with the pH of about 3.5, under axial load controlled and free corrosion potential
- Specimen electrochemically monitored via a Gamry potentiostat using Ag/AgCl reference electrode maintained at a constant distance (2 mm) from the specimen, a platinum counter electrode, and the specimen as the working electrode

Digital image correlation (DIC) technique used to measure strain

CF tests done while measuring the open circuit potential (OCP) vs. reference electrode during load-unload

<image>



Electrochemical corrosion cell made of plexiglass



CF Test Procedures



Forces and fluxes were measured under CF

- Performed CF tests for 16 samples at 87%, 80%, 70% and 57% of yield stress (460 MPa), load ratio = 0.1, loading frequency=0.04Hz
- Tests stopped after failure of specimens



Entropy Generation in CF

• Total entropy is measured from the hysteresis loops resulted from fatigue (stress-strain) and corrosion (potential-electrical) in each loading cycle





Entropic Endurance and Entropy-to-Failure

- Similarity of the total entropy-to-failure for all tests supports the entropic theory of damage proposed
- More tests needed to reduce the epistemic uncertainties and further confirm the theory





Ratio of Corrosion and Fatigue Entropies to the Total Entropy

• Reducing fatigue stress allows more time for corrosion





Thermodynamics of Damage: A Reliability Perspective

• Materials, environmental, operational and other types of variabilities in degradation forces impose uncertainties on the total entropic damage



 T_c = Current operating time; g(t) = distribution of time-to-failure, f(D|t) = distribution of damage at t

[1] Thermodynamics as a Fundamental Science of Reliability, A. Imanian, M. Modarres, Int. J. of Risk and Reliability, Vol.230(6), pp.598-608. DOI: 10.1177/1748006X16679578.(2016).



CF Life Derived From a Science-based Reliability Theorem





Conclusions

- A thermodynamic theory of damage proposed and tested
- This entropy-based damage theory forms the fundamental science supporting reliability
- This theory of damage allows for incorporation of all interacting dissipative processes in failure mechanisms
- An example of entropic-based reliability for the corrosionfatigue mechanism demonstrated application of the theory
- Other definitions of entropy based on the Shannon and the statistical mechanics entropies have equally promising applications
- Applications to PHM using data analytics methods are being pursued

Thank You!



Pictures taken on October 10. 2019





Thank you



Life of Systems Operating Far From Equilibrium

- Behavior of systems operating far from equilibrium and connected to the outside environment and strongly driven by external sources of energy could not be well predicted until recently.
- Jarzynski and Crooks showed entropy in a dissipating process, such as the cooling of a body, corresponds to the ratio: the probability that the atoms will undergo that process divided by their probability of undergoing the reverse process (which is spontaneous interaction atoms such that the body warms up)
- As entropy generation increases, so does this ratio: That is system's behavior becomes more and more "irreversible."
- This simple and rigorous formula is applicable to any dissipative process, no matter how fast or far from equilibrium

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Crooks Fluctuation

- Crooks fluctuation Theorem and Kullback-Leibler Divergence
 - Forward / reverse work distribution function related to thermodynamic work [17,18]

$$\frac{\pi_f(+W)}{\pi_r(-W)} = exp\left[\frac{W-\Delta F}{k_BT}\right] \rightarrow \Delta S_{tot} = k_B ln\left(\frac{\pi_f(+W)}{\pi_r(-W)}\right)$$

• This equation was used to find Helmholtz free energy (ΔF) [19]



Crooks Fluctuation and Jeffreys Divergence

- Crooks fluctuation Theorem and Kullback-Leibler Divergence
 - Relative entropy

$$D(\pi_f || \pi_r) = \int \pi_f(+W) \ln \frac{\pi_f(+W)}{\pi_r(-W)} dW$$

$$=\Delta S_f^{env} + \Delta S_f^{sys} + \Delta S_r^{env} + \Delta S_r^{sys} \quad (\Delta S_f^{sys} = -\Delta S_r^{sys})$$

W: work, $\pi_f(+W)$: forward work distribution, $\pi_r(-W)$: reverse work distribution, k_B : Boltzmann constant (1.381 × 10⁻²³), T: temperature, $\langle W \rangle_i$: mean work in the process i, ΔF : Helmholtz free energy difference, $\Delta \langle E \rangle_i$: mean internal energy difference in the process i, ΔS_i^{sys} : entropy change within the system, $\langle Q \rangle_i$: mean heat dissipation in the process i, ΔS_i^{env} : entropy difference dissipated to the environment in the process i, and ΔS_f^{tot} : total entropy difference in the process i



Approaches to define entropy



 k_B makes the statistical mechanics entropy equal to the classical thermodynamic entropy of Clausius

Corrosion Current vs. Potential: Effect of Time and Stress

- To obtain the correlation between *corrosion current and potential*, polarization curves were developed at different stress and immersion values
- Stress and immersion time variations showed stochastic effect on polarization curve
- The sum of the exponential terms showed a good fit to the part of polarization which involved the open circuit potential (OCP)

